

# **Turbulent Diffusion and Its Effects on the Chemistry of Molecular Clouds**

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## **ABSTRACT**

Turbulence in molecular clouds is well recognized, but the resultant diffusive transport and its effects on the chemical structure of the clouds have not been extensively investigated. We present in this article a study of the effects of turbulent diffusion using the mixing-length approximation on the chemical structure of a representative dark molecular cloud. With a diffusion term in the continuity equation for each species, we model the time-dependent gas-phase chemistry in a dense molecular cloud with fixed density and temperature profiles. We estimate the diffusion coefficient based on the observed turbulence in molecular clouds, and find that diffusive processes significantly modify the predicted chemical abundances in the dense interiors of molecular clouds, increasing the abundances for C and C<sup>+</sup> and most carbon-bearing species and lowering the abundances for some other species such as H<sub>2</sub>O and O<sub>2</sub>. These results, which can be explained in the context of the existing ion-neutral reaction scheme in terms of electron abundance changes due to diffusion, appear to agree with observations.

*Subject headings:* interstellar: abundances - interstellar: molecules  
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## 1. INTRODUCTION

Since the pioneering work of Herbst & Klemperer (1973) on a steady-state gas-phase chemistry model based on an ion-neutral reaction scheme, significant progress has been made in the chemical modeling of molecular clouds (cf. Dalgarno 1987; van Dishoeck et al. 1993). The most discussed and utilized models consider the time-dependent gas-phase chemistry of a homogeneous cloud while maintaining fixed profiles of physical parameters such as the cloud temperature and density (Prasad & Huntress 1980; Langer & Graedel 1989; Herbst & Leung 1989; Millar & Herbst 1990). The chemistry in the dense molecular gas is found to approach steady-state in a matter of millions of years or less in these models, a time scale comparable to or smaller than the age of molecular clouds (see section 3). The steady-state chemical abundances predicted by these models with normal gas-phase  $C/O$  ratio ( $C/O < 1$ ) are in general successful in accounting for the abundances for many molecular species. However, these predictions for homogeneous clouds clearly fail to explain some observations such as the observed large abundances of  $C$  (Phillips & Luggins 1981; Keene et al. 1985; Jaffe et al. 1985; Perking et al. 1989),  $C^+$  (cf. Stutzki et al. 1988; Howe et al. 1991; Stacey et al. 1993; Zhou et al. 1993),  $H_2CO$  (Federman, Huntress & Prasad 1990; Federman & Allen 1991) and of complex organic molecules (Herbst & Leung 1989) in the envelopes as well as interiors of molecular clouds. These disagreements represent some important issues in the field (Sorrel 1992) that need to be resolved in order to further understand interstellar chemistry. Mechanisms proposed to explain some of these discrepancies, in particular the large “ $C/CO$  ratio problem”, include internal photon production<sup>1</sup>, an abnormal gas-phase  $C/O$  ratio ( $C/O > 1$ , Tarafdar, Prasad & Huntress 1983; Langer et al. 1984), photodissociation regions on the surfaces of clouds or clumps (Tielens & Hollenbach 1985; Genzel et al. 1988; Zmuidzinas et al. 1988; Boissè 1990; Tauber 1990; Tauber & Goldsmith 1990; Hollenbach, Takahashi & Tielens 1991), and bistability of high  $C$  and low  $C$  phases (Le Boulouet et al. 1993; Flower et al. 1994). In addition, given the fact that the time-dependent models do produce enough  $C$  and more complex organic molecules at an “early-time” of  $\sim 10^5$  yr, significant modeling efforts have been devoted to models in which dynamical processes are expected to regulate the physical conditions, keeping the chemistry from reaching steady-state and maintaining such an “early-time” chemistry in the apparently much older molecular clouds.

One class of dynamical models considers the effects of turbulent mixing of material

<sup>1</sup>The photons can be generated by shocks (Norman & Silk 1980; Hollenbach & McKee 1989), by cosmic rays (Prasad & Tarafdar 1983), by young stars (Montemerle et al. 1983; Krolik & Kallman 1983) and even by neutrino decay (Tarafdar 1991; Sciama 1993).

between interior and exterior cloud zones, as first suggested by Phillips & Huggins (1981), and further discussed by Boland & de Jong (1982). Similar ideas were also discussed by Federman & Allen (1991) for the interpretation of the large  $H_2CO$  abundance in the envelopes of dark clouds. Computations of gas-phase chemistry including a crude transport approximation were made by Chièze & Pineau des Forêts (1989; 1990) and by Chièze, Pineau des Forêts & Herbst (1991), who considered two or three parcels of gas with mass exchange, mimicking the dense molecular gas and the diffuse molecular gas, respectively. This “artificial” mixing indeed yields chemical abundances in the dense gas parcel which are closer to the observations. The turbulent mixing approach, however, has been criticized by Williams & Hartquist (1984; 1991) based mainly on simple considerations of the turbulent transport time-scale. They argued that turbulent mixing is a diffusive process which is typically slower than the chemistry. We will show in Section 3.3 of this paper that the real situation is more complicated than they considered. As pointed out by Prasad, Heere & Tarafdar (1991), one major weakness in this class of models is the purely empirical and non-realistic treatment of the mixing processes. Indeed, Chièze, Pineau des Forêts & Herbst (1991) attempted a more sophisticated “three-stage model”, which leads to the conclusion that a continuous density variation would be needed to explain the observed large abundances of the complex organic molecules.

The second class of dynamical mixing models evokes stellar winds in a clumpy molecular clouds as suggested by Williams & Hartquist (1984) and Goldsmith, Langer & Wilson (1986). In this model, stellar winds continuously erode the dense molecular clumps, cycle the material between the clump surface and the interclump medium and keep the gas from reaching steady-state chemistry (Williams 1986; Charnley et al 1988; 1990). The third class of dynamical models includes chemistry together with gravitational collapse (cf. Gerola & Glassgold 1978; Tarafdar et al 1985; Brown, Charnley & Millar 1988; Prasad, Heere & Tarafdar 1991; Rawlings et al 1992; Hartquist et al 1993). These modeling efforts also predict molecular abundances in reasonable accord with observations, but some of them are rather complicated even under the most simplifying assumptions.

In this paper, we present a more systematic approach to the general idea of turbulent transport, which in principle allows a more realistic modeling of its effects on the chemistry in molecular clouds. We show that “turbulent diffusion”, which is theoretically expected to accompany turbulence, may offer a rather natural explanation to the “C/CO ratio problem” in the context of gas-phase chemistry. With diffusion coefficients commensurate with observed turbulence, the steady-state abundances predicted by the diffusion chemical model include larger abundances for C,  $C^+$  and other carbon-bearing species and smaller abundances for  $H_2O$  and  $O_2$  in the interior of a molecular cloud, and a smoother distribution of most species across the cloud. We start with theoretical considerations of turbulent

diffusion in the following section. We present our modeling results and analysis in Section 3. Section 4 discusses the applicability of the model, and Section 5 summarizes our conclusions.

## 2. THEORY

### 2.1. Turbulence and Diffusion

One of the well-recognized facts in molecular clouds is the almost ubiquitous presence of turbulence, as manifested by the broad line profiles of molecular tracers (Penzias 1975). Numerous theoretical and observational works have been carried out for understanding turbulent processes in molecular clouds (cf. 1 Dickman 1985; Scalo 1987; Falgarone 1989; Falgarone & Puget 1994). In contrast, little attention has been paid to the transport processes in the multi-component gas (with  $n(H_2)$  being the major component) in molecular clouds which are theoretically expected to accompany turbulence. Transport of a transferable physical quantity in random, turbulent motion is diffusive in nature.

Now assume that the highly non-linear turbulent process causes each of the gas components to move with the same random velocity  $V_t$ . Because the composition of the gas in molecular clouds may not be uniform, such a random velocity will generate fluctuations in the fractional abundance of a gas component (tracer). Unfortunately, hydrodynamics does not have an elegant theory to describe these fluctuations quantitatively. The commonly used tool in treating this physical process has been the phenomenological mixing-length theory (Hinze 1959; Lesieur 1990). This empirical theory is not really capable of describing the transport mechanisms of turbulence, but it results in a practical relationship for some useful physical quantities. The basic idea of this theory is to characterize turbulence by many moving fluid parcels (or eddies) which maintain physical properties different from those of the average fluid before traveling an average distance of  $L$  to again merge into the background fluid. The quantity  $L$  is called the mixing-length, and the turbulent transport (or diffusion) is often called eddy transport (or eddy diffusion).

As discussed in the field of atmospheric chemistry (Colegrove 1966; Hunten 1975), turbulent diffusion may be understood as the transport of gases due to turbulent mixing in the presence of composition gradients. Assume that  $n(H_2)$  is the number density of the major component,  $H_2$ , in the gas of molecular clouds,  $n_i$  is the number density of tracer  $i$ , and  $f_i = n_i/n(H_2)$  denotes the fractional abundance of the tracer  $i$ . The fluctuations in the fractional abundance  $\delta f_i$  due to the turbulence can be approximated by the product of the

composition gradient  $df_i/dz$  in the direction  $z$  and the mixing-length  $L$ ,

$$\delta f_i \sim -L \frac{df_i}{dz}. \quad (1)$$

The net transport flux of the tracer  $i$  in the  $z$  direction can be written as

$$\phi_i [cm^{-2} s^{-1}] = n(H_2) \langle V_t \delta f_i \rangle = -Kn(H_2) \frac{df_i}{dz} = -Kn_i \left( \frac{1}{n_i} \frac{dn_i}{dz} - \frac{1}{n(H_2)} \frac{dn(H_2)}{dz} \right), \quad (2)$$

where  $\langle \rangle$  denotes the time average of a quantity, and the diffusion coefficient  $K [cm^2 s^{-1}]$  is defined as

$$K = \langle V_t L \rangle. \quad (3)$$

It is clear from Eq. (2) that turbulent diffusion consists of two parts, one due to the density gradient of the tracer  $i$  and the other due to the density gradient of the major gas component  $H_2$ , respectively. Equation (2) can be re-written as

$$\phi_i = -Kn_i \left( \frac{1}{H_i} - \frac{1}{H_{H_2}} \right) = -Kn_i \frac{1}{H}, \quad (4)$$

where  $H_i = -n_i / \frac{dn_i}{dz}$  and  $H_{H_2} = -n(H_2) / \frac{dn(H_2)}{dz}$  are the density scale heights for the tracer  $i$  and  $H_2$ , respectively, and  $H = 1 / (\frac{1}{H_i} - \frac{1}{H_{H_2}})$  may be understood as the overall scale height. This expression implies that the diffusion velocity for each species is  $v_d \sim K/H$ , and thus the diffusion timescale for each species can be written as  $\tau \sim H/v_d \sim H^2/K$ .  $H$  is governed by the fractional abundance gradient, which is related to the details of the chemistry, and is highly species- and position-dependent and sensitive to other cloud conditions such as the intensity of external radiation field. 'But, the diffusion time-scale  $\tau$  is in general a complicated function, which can not be easily quantified on the scale of the cloud. Detailed chemical calculations are obviously required to obtain the fractional abundance gradient. We will defer further discussions on the diffusion time scale to Section 3.3 when we have done some numerical calculations.

## 2.2. The Turbulent Diffusion Coefficient,

To quantify the effect of the turbulent diffusion in molecular clouds, we need to estimate the diffusion coefficient  $K$ . Unfortunately, an accurate estimate of  $K$  is hampered not only by the lack of an elegant theory for turbulence, but also by the unclear nature of turbulence in molecular clouds. However, based on the observations of the turbulence in molecular clouds and the definition of  $K$  (Eq. (3)) in mixing-length theory, an order-of-magnitude:

estimate for  $K$  is possible. If we consider that the diffusion is due to the interchange of two eddies with average velocity  $V_t$  over a characteristic length scale  $L$ , Eq. (3) gives the plausible relationship  $K \sim V_t L$ .

Relatively isolated dark clouds (globules) are the type of clouds which resemble our model cloud here. For this type of cloud, Leung, Kutner & Mead (1982) found that the turbulent velocity as traced by the  $^{13}\text{CO}$  linewidths scales with cloud radius as  $V_t (\text{km s}^{-1}) = 0.58 R (\text{pc})$ . It is more difficult to relate the mixing-length  $L$  to observations since it is directly related to the unknown nature of the turbulence. However, several pieces of information allow an order-of-magnitude estimate. First, despite large optical depths,  $^{12}\text{CO}$  line profiles from these dark clouds are usually smooth and centrally-peaked, instead of "self-reversed". This property has been taken as a direct indication that the turbulence inside clouds is macroturbulence having relatively large correlation lengths (Baker 1976; Dickman 1985; Kwan & Sanders 1986). A correlation length of 10 percent of the cloud size seems to be a reasonable requirement in order to generate line profiles similar to those observed, according to these authors. A typical cloud is of a few parsecs in size, corresponding to a correlation length of a few tenths of a parsec. Second, Kleiner & Dickman (1987) applied an autocorrelation technique to observational data for the dark cloud TMC-1 and found a correlation length of  $\sim 0.1 \text{ pc}$ , which is indeed about 10 percent of the cloud size. Thus for a typical dark cloud, we may assume  $L = 0.1 - 0.5 \text{ pc}$  and  $V_t = 1 \text{ km s}^{-1}$ , resulting in  $K \sim V_t L \sim 3 \times 10^{22} - 2 \times 10^{23} \text{ cm}^2 \text{ s}^{-1}$ . Of course, if one thinks that the above  $V_t - R$  relationship also holds for each individual cloud, then one may argue that the diffusion coefficient  $K$  depends on position in individual clouds. But for the investigations in this paper, which represents a first detailed treatment of chemistry in a cloud with diffusive transport, we have decided to neglect this complication.

The turbulent mixing-length also can be estimated from a different perspective. One school of thought interprets the turbulence in molecular clouds as a manifestation of hydromagnetic waves (Arons & Max 1975; Myers & Goodman 1988; Mouschovias 1991). But given the dynamical complexity in the interstellar medium, there is little reason to believe that the waves are completely coherent and non-interrupted. Interrupted, non-coherent wave motion will also cause diffusive transport, which may be approximated by the mixing-length theory. In this case, the mixing-length is roughly the wavelength  $\lambda$  of the wave motion (Huntén 1975), and thus  $K \sim V \lambda$ . The wave velocity  $V$  is indicated by the observed turbulent velocity  $V_t$ . A lower limit to the wavelength of the wave motion can be obtained by considering the minimum wavelength for which ions and neutrals are closely coupled together by collisions; for typical physical conditions in molecular clouds,  $\lambda_{\min} \sim 0.1 \text{ pc}$  (Arons & Max 1975; Pudritz & Carlberg 1988), in agreement with that estimated above. Overall, we feel that the turbulent velocity is a quantity well constrained

by observed spectral linewidths, and its uncertainty is relatively small. On the other hand, there is a larger uncertainty in the estimate of  $K$  due to our lack of detailed knowledge of the mixing-length. Given the above analysis, it is relatively safe to conclude that  $K$  is on the order of  $\sim 10^{23} \text{ cm}^2 \text{ s}^{-1}$  for a majority of dark molecular clouds.

### 2.3. The Cloud Model and the Chemistry Network

In this paper we concentrate on a description of our methodology and some major results for simple molecules. Our treatment is also limited to a simple cloud model. We define our cloud to be an isothermal sphere having a constant kinetic temperature of 10 K and a density profile of  $n_{H_2}(r) = n_0 \frac{r_0}{r}$  where  $n_0 = 8.8 \times 10^2 \text{ cm}^{-3}$  is the molecular hydrogen density at the cloud boundary  $r_0 = 1.11 \text{ pc} = 3.41 \times 10^{18} \text{ cm}$ . This  $r_0$  is adopted so that the cloud has a total visual extinction of 24 magnitudes towards the center, corresponding to a total column density of  $\sim 2.4 \times 10^{22} \text{ H}_2 \text{ cm}^{-2}$ . The total mass of the cloud is  $M = 340 M_\odot$ . The cloud is assumed to be subject to a typical interstellar radiation field as discussed by Viala (1986), but we assume that the gas throughout the cloud has a kinetic temperature of 10 K (no effort was made to solve for the kinetic temperature by considering the thermal balance between cooling and heating processes).

The chemistry network (Viala 1986) includes 87 atomic and molecular species and some 1100 chemical reactions, including photo-destruction processes. In this paper we do not consider isotopic species. Given our primary aim to investigate the effects of turbulent diffusion on the gas-phase chemistry, we have made no attempts to include gas-dust interactions (cf. Duley 1989). We do not include sulfur chemistry except for the balance between S and  $S^+$ , but intend to include sulfur chemistry in a future work. For the dissociative recombination rate coefficient of  $H_3^+$ , we have used  $1.5 \times 10^{-7} (T/300)^{-0.5} \text{ cm}^3 \text{ s}^{-1}$  (Canosa et al 1991; Bates, Guest & Kendall 1993). This rate coefficient is very close to the most recent value of  $1.15 \times 10^{-7} (T/300)^{-0.65} \text{ cm}^3 \text{ s}^{-1}$  (Sundström et al 1994). The cosmic ray ionization rate is taken to be  $4 \times 10^{-17} \text{ s}^{-1} \text{ H}_2^{-1}$ , but our results in this paper are not sensitive to its exact value within a factor of a few.

With a transport term, the continuity equations that describe a time dependent chemistry of a molecular cloud are

$$\frac{\partial n_i}{\partial t} + \frac{\partial \phi_i}{\partial z} = P_i - L_i \quad (5)$$

where  $P_i$  and  $L_i$  are the production and loss terms for tracer  $i$ . A computer program to solve the coupled continuity equations, one for each species other than  $He$  and  $H_2$ , which were

not allowed to vary, was developed for modeling the chemistry of planetary atmospheres (Allen, Yung & Waters 1981). We have utilized this code to model the time-dependent gas-phase chemistry of molecular clouds with fixed temperature and density profiles.

The initial gas-phase elemental abundances used are tabulated in Table 1. Initial abundances for all other species are assumed to be 0. We have no direct measurement of their abundance and our knowledge of the metal depletion in interstellar clouds is not very good. We have adopted a depletion factor of three orders of magnitude for *Mg*, *Si* and *Fe* in our standard model, which is roughly an order of magnitude larger depletion than that found for diffuse clouds (c.f. Leger, Jura & Omont 1985; Joseph et al. 1986; Bergin, Langer & Goldsmith 1994). Since we have not included sulfur chemistry in our network, the low abundance used for S is based on the modeling results that sulfur should be mostly locked up in sulfur molecules even if the depletion is smaller (Herbst & Leung 1989; Millar & Herbst 1990). Assuming that the cloud is relatively isolated, we require that the turbulent diffusion fluxes  $\phi_i$  at the boundaries be zero for all species.

We adopt a 1-1) geometry to simplify the radiative transfer and the turbulent diffusion. We also follow the methodology of Viala (1986) in the treatment of continuum attenuation of the UV radiation. We do not include the  $H_2$  self-shielding, but we take into account the CO self-shielding by scaling the CO photo-dissociation rate by a factor at every time step. This scaling factor is estimated according to the CO self-absorption values as calculated and tabulated in van Dishoeck & Black (1988) by means of spline interpolation (cf. Bergin, Langer & Goldsmith 1994). Our decision to avoid treating the formation of molecular hydrogen is based on the major objective of this paper to investigate the effects of turbulent diffusion on the chemistry of minor species other than  $H_2$  in dense molecular regions.

We calculate the chemical abundances at 22 grid points of different radii in the cloud. The properties of the grid points are listed in Table 2.

### 3. DIFFUSION CHEMISTRY

#### 3.1. Results

Figure 1 presents the evolution of species abundances as a function of time in the grid point at  $r \leq 1 \times 10^{17}$  cm with a density  $n(H_2) = 3 \times 10^4$  cm<sup>-3</sup> and a visual extinction of 9 magnitudes from the boundary. The solid curve shows the chemistry without diffusion, and the other two curves show the abundance variations with two different diffusion coefficients,  $K = 1023$  cm<sup>2</sup> s<sup>-1</sup> and  $K = 1024$  cm<sup>2</sup> s<sup>-1</sup>, representing the typical value and the upper



Table 1: Initial Elemental Fractional Abundances

Species	$n(x)/n(H_2)$
$H_2$	1
$He$	0.22
$N$	$7.30 \times 10^{-5}$
$O$	$1.70 \times 10^{-4}$
$C^+$	$1.00 \times 10^{-4}$
$S^+$	$1.60 \times 10^{-8}$
$Mg^+$	$3.40 \times 10^{-8}$
$Si^+$	$3.40 \times 10^{-8}$
$Fe^+$	$2.00 \times 10^{-8}$

Table 2: Grid Properties of the Cloud Model

Grid	Radius $R$ (cm)	$n(H_2)(cm^{-3})$	$A_v(R)$ (magnitude)
1	$1.00E+17$	$3.00E+04$	9.00
2	$1.50E+17$	$2.00E+04$	8.00
3	$2.25E+17$	$1.33E+04$	7.00
4	$3.38E+17$	$8.89E+03$	6.00
5	$5.06E+17$	$5.92E+03$	5.00
6	$7.59E+17$	$3.95E+03$	4.00
7	$1.14E+18$	$2.63E+03$	3.00
8	$1.71E+18$	$1.76E+03$	2.00
9	$1.90E+18$	$1.58E+03$	1.70
10	$2.11E+18$	$1.42E+03$	1.40
11	$2.34E+18$	$1.28E+03$	1.10
12	$2.51E+18$	$1.19E+03$	0.90
13	$2.69E+18$	$1.12E+03$	0.70
14	$2.78E+18$	$1.08E+03$	0.60
15	$2.88E+18$	$1.04E+03$	0.50
16	$2.98E+18$	$1.01E+03$	0.40
17	$3.08E+18$	$9.74E+02$	0.30
18	$3.19E+18$	$9.41E+02$	0.20
19	$3.30E+18$	$9.10E+02$	0.10
20	$3.33E+18$	$9.00E+02$	0.07
21	$3.38E+18$	$8.89E+02$	0.03
22	$3.41E+18$	$8.88E+02$	0.00

limit respectively. As this paper is intended to illustrate the effects of turbulence, we have plotted only some simple, carbon-bearing and the oxygen-bearing species. These have been chosen either because they are observationally relevant or because they are major reservoirs of oxygen atoms. While the abundances for most species change as a function of time, each of them approaches a constant in a few million years, which we call steady-state in this paper. Diffusion leads to significant changes to the ‘(steady-state)’ abundances of some ‘diffusion-sensitive’ species, including the simple, common species such as C,  $O_2$ ,  $H_2O$ ,  $CH$ ,  $C_2H$  and  $H_2CO$ . Other species, including CO and OH, are less sensitive to diffusion, and their abundances only undergo minor modifications. With strong turbulent diffusion (e.g.,  $K = 10^{24} \text{ cm}^2 \text{ s}^{-1}$ ), the abundance of C at early-time ( $\sim 10^5$  years) is essentially maintained as a steady-state value. Unlike C, the steady-state abundances of  $H_2O$  and  $O_2$  are predicted to decrease with increasing strength of the turbulent diffusion.

Figure 2 displays the abundance variations at steady-state as a function of cloud radius. Again, the solid curve is calculated without diffusion, and other curves are the calculations for different diffusion coefficients. Given the fact that we did not take into account the self-shielding of  $H_2$  and assumed the gas has a kinetic temperature of 10 K without examining its thermal structure, the chemical abundances at the boundary layers ( $A_v \leq 0.5 \text{ mag}$  or  $R > 2.8 \times 10^{18} \text{ cm} = 0.9 \text{ pc}$ ) are probably incorrect. Our qualitative results and conclusions are based on the comparison between the diffusion and non-diffusion case. An important effect of turbulent diffusion is that it smears out almost all of the ‘sudden’ changes in the abundance variations as a function of radius, resulting in smoother radial profiles for almost all species. This smoothing is due to the fact that diffusion tends to reduce the gradients of the fractional abundances. CO is relatively constant throughout the cloud with or without diffusion; C also can be a very uniform tracer of the gas under diffusion. A prediction of the diffusion model is that atoms and atomic ions such as C and  $C^+$  have larger abundances in the interior of the clouds and permeate the whole cloud. The fractional abundance of C in the center in particular increases by 3 orders of magnitude when  $K$  increases from 0 to  $10^{23} \text{ cm}^2 \text{ s}^{-1}$ , and increases by another order of magnitude for  $K = 10^{24} \text{ cm}^2 \text{ s}^{-1}$ . But even with very strong turbulence, the fractional abundance of  $C^+$  has a very significant radial gradient because of its sensitivity to the UV radiation field.

As column density (not the volume density) is usually the directly observable physical quantity, we have also calculated the steady-state column densities for some key species as a function of offset from cloud center. Figure 3 presents the calculations as fractional column densities relative to CO. The effects of turbulent diffusion are obvious. Table 3 presents a comparison of the fractional abundances calculated towards the cloud center for some simple carbon-bearing and oxygen-bearing species predicted by our model and those observed in a few molecular clouds. It is useful to point out that the C/CO ratio in terms

Table 3: Comparison of Model Results with Observations

Species	Observed $N(X)/N(H_2)$				Model $N(X)/N(H_2)$ at Steady State			
	TMC1	"ref."	1.134N	"ref."	$K = 0$	$K = 10^{22}$	$K = 10^{23}$	$K = 10^{24}$
co"	8(-5)	IGH	8(-5)"	IGH	9.0(-5)	9.0(-5)"	8.3(-5)	4.4(-5)
c / c o	$\geq 0.1$	SKLPR	$\geq 0.1$	PH	0.02	0.02	0.09	0.9
$C^+$					7.5(-6)	7.8(-6)	9.2(-6)	1.4(-5)
$C_2$	5(-8)	IGH			2.0(-8)	2.6(-8)	7.8(-8)	5.1(-7)
CH	2(-8)	IGH	1(-8)	IGH	6.6(-8)	7.5(-8)	1.2(-7)	2.4(-7)
$C_2H$	5(-8)	IGH	< 5(-8)	IGH	9.4(-9)	1.3(-8)	3.5(-8)	1.3(-7)
$O_2$			$\leq 1(-5)$	PLC	6.5(-6)	3.4(-6)	6.4(-7)	2.8(-8)
OH	3(-7)	IGH	7(-8)	IGH	7.1(-8)	6.3(-8)	4.6(-8)	1.2(-8)
$H_2O$	< 1(-5)	LG			2.3(-7)	1.8(-7)	4.9(-8)	1.0(-9)
$HCO^+$	8(-9)	IGH	8(-9)	IGH	2.9(-9)	2.5(-9)	1.1(-9)	4.1(-11)
$H_2CO$	2(-8)	IGH	2(-8)	IGH	7.3(-9)	1.3(-8)	2.7(-8)	6.2(-9)

Note. - IGH, Irvine, Goldsmith & Hjalmarsen (1987); LG, Langer & Gracel (1989); PH, Phillips & Huggins (1981); PLC, Pagani, Langer & Castets 1993 the detection is tentative and the abundance estimate is highly uncertain; SKLPR, Schilke et al (1994)

of column density does not seem to be changed by diffusion as much as that in terms of density because of the contribution of the C abundance in outer layers of the cloud, which is not very sensitive to diffusion. In fact, the NON is as high as  $\sim 0.02$  without diffusion, not as terrible a discrepancy from the observed value of  $\sim 0.1$  as some authors claimed based on modeled values for  $n(C)/n(CO)$ . This point was noticed and discussed by Viala (1986). However, it is conceivable that a more massive cloud with a denser core and a larger column density will have a much smaller  $N(C)/N(CO)$  in the no-diffusion case, and the discrepancy between the model results without diffusion and the observations will be correspondingly larger.

in general, turbulent diffusion makes significant changes to the radial distributions in the steady-state. For  $K \sim 1023 \text{ cm}^2 \text{ s}^{-1}$ , the steady-state value of  $\sim 0.1$  for the  $N(C)/N(CO)$  ratio is consistent with observations for a variety of molecular clouds (cf. Phillips & Huggins 1981; Keene et al 1985; Schilke et al 1994). A  $C/CO$  ratio close to 1 is obtained for stronger turbulence, say  $K = 1024 \text{ cm}^2 \text{ s}^{-1}$ . The radial profiles of  $C$  and  $C^+$  are modified significantly by diffusion and they appear to have relatively large abundances even in the interior of the cloud. The "steady-state" abundances for other important chemical species, including  $C_2$ ,  $CH$ ,  $C_2H$ ,  $OH$  and  $H_2CO$ , predicted by our model for  $K \sim 10^{23} \text{ cm}^2 \text{ s}^{-1}$  are in overall agreement with observations, as shown by Table 3. For most species, the abundances increase or decrease *monotonically* with increasing  $K$  within the range tested, but an exception occurs for  $H_2CO$ , whose abundance first increases with increasing  $K$ , and then starts to decrease at a  $K$  value above  $\sim 1023 \text{ cm}^2 \text{ s}^{-1}$ . The predicted abundances for both  $H_2O$  and  $O_2$  for the no-diffusion case are below the upper limits established by most observations of hotter and more massive clouds (cf. Combes et al. 1991; Phillips, van Dishoeck & Keene 1992), and further decrease monotonically with increasing  $K$ . Oxygen has also been searched for via the  $^{16}O^{18}O$  isotope in dark clouds (Fuente et al. 1993; Pagani, Langer & Castets 1993) similar to the cloud modeled here. In only one source, L134N, is there a tentative detection at about the  $3\sigma$  level (Pagani et al. 1993) and the  $O_2/CO$  ratio is estimated to be  $\sim 0.1$  (Pagani, Langer & Castets 1994). On face value, it is consistent only with a weak diffusion case. The tentative nature of the detection and the uncertainties in estimating its abundance, however, preclude making any strong conclusions at this time. In all other dark clouds only upper limits for  $O_2/CO$  have been established; less than 0.1 to 0.2 for B5 and TMC2, for example. These limits are consistent with our models with  $K > 0$  but are not good to be enough to be used for any detailed comparison.  $K \sim 10^{23} \text{ cm}^2 \text{ s}^{-1}$  leads to abundances in good agreement with observations for  $H_2CO$ ,  $C_2$  and  $C_2H$ . The predicted abundances for  $OH$  with  $K$  from 0 to  $1024 \text{ cm}^2 \text{ s}^{-1}$  and for  $HCO^+$  with  $K$  from 0 to  $1023 \text{ cm}^2 \text{ s}^{-1}$  agree with the observations within an order of magnitude, while  $K = 1024 \text{ cm}^2 \text{ s}^{-1}$  leads to far too low an abundance for

$HCO^+$ . The  $HCO^+$  abundance is particularly sensitive to the electron abundance, roughly as  $x(e)^{-2}$ , because its destruction by recombination and production by reactions with  $H_3^+$  are sensitive to the electron abundance. For  $K = 0$  the metal abundance controls the ionization balance in the innermost layers as most of the ions are in the form of  $Mg^+$ ,  $Fe^+$  etc. A smaller gas-phase metal abundance (i.e., a larger depletion) will increase the electron abundance, which will increase the predicted abundance for  $HCO^+$  and slightly decrease the  $C/CO$  ratio as well. However, with larger  $K$   $H^+$  and  $C^+$  become more important for the ionization balance in the interior.

Finally, we have carried out an investigation to see how sensitive the diffusion chemical model is to the initial chemical abundances and how it responds to sudden changes of the dynamical state (e.g. changes in turbulence) under the same set of gas-phase elemental abundances. We first allowed the chemistry to evolve without diffusion until it attained steady state, and then we turned on diffusion. The chemistry adjusted itself to achieve the same steady state within the same time-scale as it would have had starting from non-molecular initial conditions with the same diffusion coefficient  $K$ . We then turned off the diffusion, and then the chemistry recovered to the same steady state that it achieved when starting from purely atomic initial conditions without diffusion. We have also tried to change the diffusion coefficient before the majority of the chemical species attain steady-state abundances. All the tests show that the steady-state gas-phase abundances are not sensitive to the initial physical conditions. As long as the gas-phase elemental abundances stay the same, the chemistry adjusts itself within a certain time to achieve a unique chemical steady state. The timescale of the adjustment is determined by the terminal dynamical state. The chemical timescale is largest when the diffusion is turned off ( $K = 0$ ). The above tests, albeit naive in maintaining the same cloud structure while changing the turbulent state of the cloud, imply that the observed chemistry might to some degree reflect the dynamical state of a cloud, or vice versa, since the timescale for adjustment is typically shorter than the lifetimes of molecular clouds. Of course, the real situation could be much more complicated than this. It is conceivable that when one or more young stellar objects emerge in a cloud which is in a quasi-static state on a global scale, stellar winds may change the turbulent state of the cloud. If the cloud quickly adjusts its dynamical state and stays in the same dynamical state over a timescale longer than the chemistry timescale, then the cloud can be approximated as "quasi-static" and the chemistry will have enough time to attain its steady state. If the dynamical response time of the cloud is longer than the chemistry timescale, then the cloud cannot be modeled as "quasi-static" for chemical studies, and the chemistry may never achieve its steady state. This latter situation is similar to what is considered by the stellar wind erosion chemical models and free-fall collapse chemical models.

### 3.2. Why Diffusion Modifies the Chemistry

The behavior of the chemistry discussed above, i.e., sensitivity to the diffusion coefficient, can be understood in terms of electron abundance changes, which are determined by several main factors including the cosmic ray intensity, the radiation field, metal abundances, and in particular the turbulent diffusion term. The electron abundance is reflected through the relative importance of several ions, such as  $H^+$ ,  $He^+$ ,  $H_3^+$  and  $C^+$  as well as metal ions. In dense UV-shielded interiors of clouds, ions are mainly produced by the ionization of molecular hydrogen and subsequent charge transfer from hydrogen ions ( $H^+$  and  $H_3^+$ ) to other species. Although the ion production rate by this cosmic ray ionization is independent of the density, the rate that they recombine is sensitive to the electron density. The electron abundance usually decreases with increasing density, but diffusion can play a major role in changing the electron abundance in the interior of clouds by transporting in electrons and ions from outer layers.

The results for the non-diffusion case ( $K = 0$ ) correspond very well to those produced by previous models of time-dependent chemistry with static cloud structure. The behavior with respect to the radiation field and ionization has been discussed in detail by a number of authors and here we only touch on the key points. In the radiation-dominated outer regions of the cloud, the carbon ions initiate the carbon chemistry through the radiative association reaction,  $C^+ + H_2 \rightarrow CH_2^+ + h\nu$ , and the ionization is sustained mainly by the UV radiation field. Oxygen-based molecules (e.g.,  $OH$ ,  $O_2$  and  $H_2O$ ) can be formed from  $O^+$  reacting with  $H_2$  but the  $O^+$  is produced mainly by charge exchange with  $H^+$  (as the reaction is endothermic, it occurs mainly in warm gas with  $T > 40$  K, which is not considered by the model presented in this paper). The balance between atomic and molecular form is mainly a competition between production by these ion-neutral reactions and photodestruction by the radiation field. However, in the absence of any other chemical mechanisms these trace molecules do not survive in the deep UV-shielded cold interior, because the production mechanisms shut down while cosmic ray-produced helium ions sustain destruction.

In the UV-shielded interior of a cloud it is the buildup of the  $H_3^+$  ion and the subsequent production of molecular ions (e.g.,  $OH^+$  and  $CH^+$ ) that is responsible for the formation of molecules and an active carbon and oxygen gas-phase chemistry through protonation reactions. The molecules, nevertheless, are subject to destruction by ions such as  $C^+$ ,  $H^+$  and  $He^+$  etc. The  $C^+$  recycle  $O_2$  and  $H_2O$  into carbon compounds (e.g.,  $HCO^+$  and  $CO$ ). Charge transfer reactions with  $H^+$  tend to be more dominant than with  $He^+$  in removing  $O_2$  and  $H_2O$  partly because of the larger abundance of  $H^+$  and larger reaction rate. But  $He^+$  is essential in keeping carbon from being all locked up in  $CO$  and keeping the carbon chemistry alive (Langer 1976; Graedel, Langer & Prerking 1982). It is the balance between

these production and destruction mechanisms that determines the chemistry. The balance depends to first order on the electron abundance mainly through the sensitivity of  $H_3^+$  ion abundance to electron recombination. The balance is indirectly sensitive to the cosmic ray ionization rate through its influence on the electron abundance. Typically the fractional abundance of electrons must be above a certain value,  $x(e) \sim 10^{-6}$ , to have a complete conversion of oxygen and carbon into molecular form in the shielded interiors.

This sensitivity of chemistry to the electron abundance in the interior of a cloud leads to two different equilibrium phases or regimes, depending on the physical conditions. The chemistry switches non-linearly and quasi-discontinuously from one phase to the other due to the nature of the coupling between electron, ion and molecular abundances. The two phases and the switch-over between these two phases as a result of density change can be seen clearly in the figures of Grardel et al. (1982) where the oxygen chemistry changes suddenly within a small density range. The existence and importance of these two phases have recently been emphasized and further demonstrated by Pineau des Forêts, Roueff & Flower (1992) and Flower et al (1994). Le Bourlot et al (1993) found that the transition zone between the two phases (which they called high and low ionization phases or HIP and LIP, respectively) is bistable within a relatively small range of physical conditions. The two phases and the phase transition can be understood qualitatively in terms of relative importance of  $H^+$  and  $H_3^+$ . Suppose now at a high density the chemistry is maintained at LIP phase with abundant saturated molecules such as  $H_2O$  and  $O_2$  due to the large abundance of  $H_3^+$ . In this phase, the abundances of C and C atoms will be small because  $C^+$  is removed by  $H_2O$  and  $O_2$ . When the density drops, the fractional abundances of  $H^+$  and electrons rise, followed by a reduction of the  $H_3^+$  abundance. The reduction of  $H_3^+$  will then cause a decrease in the production of  $H_2O$  and  $O_2$ , which are the principal removers of  $H^+$  and  $He^+$ . Thus, high abundances of  $H^+$  and  $He^+$  will be achieved, and there will be less  $H_2O$  and  $O_2$  and subsequently more C and  $C^+$ . Pineau des Forêts, Roueff & Flower (1992) concluded that the quasi-discontinuous transition occurs when  $H_3^+$  is as rapidly removed by its recombination with  $e^-$  as by its protonation with neutrals such as CO and O.

The two phases and the quasi-discontinuous phase transition seem to appear also in our non-diffusion case ( $K = 0$ ) as seen in radial profiles shown in Figure 2. The majority of the species undergo a sudden change at  $R \sim 7 \times 10^{17} \text{ cm}$ , corresponding to a density of  $n(H_2) \sim 4 \times 10^3 \text{ cm}^{-3}$  which is close to the value  $2.75 \times 10^3 \text{ cm}^{-3}$  reported by Pineau des Forêts, Roueff & Flower (1992). In fact, a similar mechanism may explain the quasi-discontinuous change in chemical abundance in the time evolution of the chemistry (see Figure 1) just before attaining the steady-state. Finally, it is noteworthy that a second phase jump occurs at an outer radius ( $R \sim 2.5 \times 10^{18} \text{ cm}$ ), which separates the

radiation-dominated chemistry and the regular dense cloud chemistry, as seen in many previous studies of photo-dissociation regions (cf. Langer 1976; Viala 1986; Hollenbach, Takahashi & Tielens 1991).

With the above understanding about the sensitivity of the chemistry to the electron abundance and the existence of the two phases in the dense cloud chemistry, it is now possible to understand qualitatively the results of the diffusion chemistry ( $K > 0$ ). The diffusion term transports material radially in the cloud, depending on the fractional abundance gradient. As can be seen in the results for  $K > 0$  there is a net transport of  $C^+$ ,  $H^+$ ,  $He^+$  and other ions from the outer layers to the inner layers of the cloud. This transport results in an increase in the electron abundance in the interior and at some critical point the high ionization phase discussed by Le Bourlot et al. (1993) is attained throughout the UV-shielded interior of the cloud. In this case the higher abundances of electrons and ions such as  $H^+$  and  $He^+$  suppress the abundances of  $H_3^+$ ,  $H_2O$ ,  $O_2$  and even  $CO$ , and enhances the abundances of  $C$ ,  $C^+$ ,  $CH^+$  and other carbon-bearing species. The stronger the diffusive transport, the more carbon and carbon-bearing species, and the less  $H_2O$  and  $O_2$  will be generated in the interior of the cloud. Although the chemistry in the outer photo-dissociation region is less affected by the diffusive transport, the quasi-discontinuous changes of the chemical abundances across the cloud are effectively smeared out by the diffusion.

### 3.3. Time Scales

As mentioned in the introduction, one of the criticisms that Williams & Hartquist (1984; 1991) made of the turbulent mixing concept was based on the consideration that the estimated transport time-scale over a cloud is  $R^2/LV_t$ , which is far larger than typical chemical time scales of concern. These authors were correct in that the time scale for diffusion is not  $\sim \frac{R}{V_t}$ , where  $R$  is the radius of the cloud. However, the turbulent transport time-scale  $\tau \sim H^2/K$  (see Section 2.1) depends on the composition gradient of a specific tracer, which depends on the density scale heights of both the concerned species and  $H_2$ . It is important to realize the importance of both density scale heights,  $H_i$  and  $H_{H_2}$ . For example, it is not unusual for a species to have a roughly constant fractional abundance within a certain range of radius in the cloud, as can be seen from the solid curves in Figure 2. In this case we should expect little diffusion. Yet since the second term  $1/H_{H_2}$  in Equation (3) is never zero in the adopted cloud model, the first term must be nearly as large within the radius range in order to cancel the second term. In general, the diffusion time scale at a position can be rather complex even if  $K$  is assumed constant throughout the cloud, as can be seen from Equations (2) and (3). The transport becomes species-independent



only when  $H_i$  becomes infinitely large, but even in this case the transport timescale is still position dependent, and may not be related to the time constant  $R^2/K$  in any rigorous manner on the scale of the cloud. That is to say that the diffusion can not be understood as merely a mixing between the boundary layer and the center of the cloud, although the chemical difference is usually the largest between the very center and the boundary of the cloud. Imagine that the cloud consists of many zones of noticeably different chemical compositions and physical conditions at a particular time. The diffusive transport between two neighboring zones will occur if there exists a composition gradient between the two zones. As long as the transport timescale between two such neighboring zones is comparable to or shorter than the time-scale of the chemistry, the chemistry will be closely coupled to the diffusion processes, especially when the chemistry is sensitive to small changes of some key species as discussed earlier in this paper.

The approach to compare the diffusion and timescales may be a valid idea, but in reality both time scales are highly species as well as position dependent, and an adequate comparison of the two timescales requires a detailed numerical solution to Equation (5). We conclude that the diffusion coefficient  $K$  should be taken as the basic parameter to characterize the diffusion. The time constant " $R^2/K$ " should be interpreted with caution as an upper limit for the real diffusion timescale. This point can be seen from the modeling calculations presented in Figure 1. Most species attain each steady state in a time interval of  $\sim 10^6$  years, which can be roughly regarded as the chemical timescale  $\tau_{chem}$ . This chemical timescale is comparable or even smaller than the time constant  $R^2/K = 3 \times 10^6$  years for the modeled cloud. Yet the diffusion drastically modifies the chemical abundances and radial distributions of many important species, as shown in Figure 2.

## 4. DISCUSSION

### 4.1. Applicability of the Chemical Diffusion Model

Interstellar chemistry is based on the assumption that molecular clouds originate from neutral clouds whose gas is initially in atomic form. Thus, the applicability of the time-dependent chemical modeling to observations depends on the dynamical evolution and ages of molecular clouds. Although the age for molecular clouds is still a rather controversial issue (cf. Blitz & Shu 1980; Scoville & Sanders 1987; Kwan 1988; Elmegreen 1991), the lower limit for the age of many clouds seems to be on the order of  $10^7$  years, based on the ages of low-mass stars which are still embedded in molecular clouds. This age is comparable to or larger than the time that it takes for the chemistry to reach steady state under typical

fixed physical conditions (e.g. density and temperature), as mentioned in the Introduction. Thus from this argument alone, the “steady-state” abundances appear more relevant to the observations of the molecular clouds.

Our approach in this article does not explicitly include star forming processes, but the assumption of dynamical mixing is not sensitive to the exact origin and nature of the turbulence (Chièze & Pineau des Forêts 1989, 1990; Chièze, Pineau des Forêts & Herbst 1991). The turbulence can be a result of stellar winds, differential cloud rotation, magnetic waves, slow gravitational contraction, thermal instabilities or Kolmogorov eddy cascades (cf. Dickman 1985; Scalo 1987; Myers 1987). If the impact from young stellar objects on molecular clouds is limited to the generation of turbulence to the zeroth order (Norman & Silk 1980; Silk 1989), then the turbulent diffusion model may also be applicable semi-quantitatively to low-mass star forming dense clouds as a whole. The fact that most molecular clouds as a whole are supported and roughly virialized with internal turbulent motion (Larson 1981; Shu, Adams and Lizano 1987; Silk 1989) seems to lend strong support to the quasi-static assumption. Of course, this assumption is more questionable in the local neighborhood of young stellar objects, where the special dynamical effects due to star formation may be dominant (Mundy, Wootten & Wilking 1990; Herbst 1990; Blake, van Dishoeck & Sargent 1992).

Our work presented in this paper does not consider gas-dust interactions (depletion and desorption processes in particular) which can be very important, depending on the physical conditions in the cloud (cf. Caselli, Hasegawa & Herbst 1993; Bergin, Langer & Goldsmith 1994). This simplification is desired in this investigation for the sake of concentrating on the effects of turbulence in the gas-phase ion-neutral reaction scheme. Yet, it is curious what will be the effects of grains (small grains such as PAHs in particular) on the chemical diffusion model (I. Hollenbach, private communication). We hope that detailed approaches to this issue will consist our next paper on this subject.

In general, although the model presented in this paper is oversimplified in several aspects, the problems that we attempted to address are relatively well defined within the time-dependent gas-phase chemistry regime with static cloud structure, and some of the dynamical effects of low-mass star formation might be implicitly included in the treatment of turbulent diffusion. Further, given the evidence that the majority of molecular clouds are in apparent virial equilibrium as a whole, despite star formation on smaller scales, the chemical modeling presented in this paper may still be relevant to molecular clouds with low-mass star formation]. For turbulent dark clouds such as TMC-1 and L134N where no significant star formation is known to have occurred and there is no evidence for rapid global gravitational collapse, our model seems to be particularly relevant. Finally, it is

conceivable that the significantly enhanced abundances for  $C$  and  $C^+$  will lead to enhanced abundances for complex organic molecules as discussed by Chièze, Pineau des Forêts & Herbst (1991). We defer our treatment of this problem to a future paper.

#### 4.2. Some Implications of the Model

As discussed in the previous section, the key reason why the diffusion modifies the chemistry in the interior of the cloud is the change in electron abundance and ion abundances. This can be understood in that the ion-neutral reaction scheme is the basic reason why molecules are abundant in the low temperature interiors of dense molecular clouds. Most of the models proposed to explain the large abundance of atomic carbon, as summarized in the introduction, are related more or less to the abundances of electrons and ions. In comparison to the models where ionization or dissociation by external UV photons or by cosmic ray-induced UV photons, diffusion supplies ions and electrons to the chemistry in the shielded interior by shifting what is available from outer layers instead of producing them locally. In other words, instead of the penetration of UV radiation (cf. Boissè 1990 and Tauber & Goldsmith 1990) and cosmic rays (Prasad & Tarafdar 1983), in our present model the ions and other species diffuse in. Yet, there are major differences. One difference is that regions having different physical conditions are now coupled chemically in this diffusion model. The second is that the predicted radial profiles of the abundances for most species under diffusive conditions are much smoother. This is particularly true for  $C$  and  $CO$ , whose fractional abundances are mostly uniform across the cloud except at the very surface. Thus in this sense, both  $CO$  and  $C$  could be reliable tracers of the column densities under the common-used assumption of constant fractional abundances across the cloud. A carefully designed observational study of the radial profiles of some selected species may provide useful tests of the diffusion model proposed in this paper.

As our model results have shown, the  $C/CO$  ratio is dependent on the strength of the turbulence. Thus, one prediction of our model is that  $C/CO$  ratio in different molecular clouds may to some degree be correlated with the linewidths of gas tracers. If the turbulence is related to the stellar winds or bipolar outflows, then a correlation trend of the average  $C^0/CO$  ratio with the mechanical luminosity may be expected too. Unfortunately, the commonly observed lines for  $C$  and  $CO$  are all optically thick, and the large uncertainties in the determination of their column densities (cf. Walker et al 1993; Cho et al 1994) preclude such a study at present. But since the same trend should also be true for other simple carbon-bearing species, careful selection of optically thin lines from organic species may be helpful. Likewise, an anti-correlation may be expected for the abundances of  $O_2$  and  $H_2O$  with the strength of turbulence.

## 5. SUMMARY

We studied turbulent diffusion and its effects on the chemical modeling of molecular clouds, and argued that diffusive fluctuations in the gas composition are a natural consequence of turbulence. We estimated the magnitude of the diffusion coefficient in molecular clouds in the context of the phenomenological mixing-length theory, and included a diffusion transport term in the continuity equations of the chemistry network and investigated the effects of diffusion on the chemistry by considering a dense cloud which has fixed profiles of density and temperature and is subject externally to the average interstellar radiation field.

Our calculations have shown that diffusion processes significantly modify the "steady-state" abundances and radial profiles of some important species in the framework of the commonly-used time-dependent chemistry with static cloud structure. Very notable are the predicted "steady-state" abundances of  $C$ ,  $O_2$  and  $H_2O$  in the interior of the dense cloud under diffusive conditions, which are in better agreement with observations than those previously obtained. We thus suggest that, with the inclusion of diffusion processes which are expected to accompany the turbulence observed in molecular clouds, the widely-used time-dependent chemistry networks can satisfactorily account for some of the problems encountered in previous theoretical models of the interstellar chemistry.

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### Figure Captions

Figure 1. The time evolution of the chemistry at the grid point with  $A_v = 9 \text{ mag}$  and  $n(H_2) = 3 \times 10^4 \text{ cm}^{-3}$  under different diffusion coefficients. The solid curve is for the no-diffusion case, the dashed curve is for  $K = 10^{23} \text{ cm}^2 \text{ s}^{-1}$  and the dotted curve is for  $K = 10^{24} \text{ cm}^2 \text{ s}^{-1}$ .  $M^+$  denotes the sum of metal ions, including  $S^+$ ,  $Mg^+$ ,  $Si^+$  and  $Fe^+$ .

Figure 2. The radial distributions of the fractional abundances at steady-state (at a time larger than  $\sim 3 \times 10^6$  years in this case) for some simple, carbon- and oxygen-bearing species. The solid curve is for the no-diffusion case, the dashed curve is for  $K = 10^{23} \text{ cm}^2 \text{ s}^{-1}$  and the dotted curve is for  $K = 10^{24} \text{ cm}^2 \text{ s}^{-1}$ .  $M^+$  denotes the sum of metal ions, including  $S^+$ ,  $Mg^+$ ,  $Si^+$  and  $Fe^+$ .

Figure 3. This figure shows the column densities of  $C$ ,  $H_2CO$  and  $HCO^+$  with respect to the column density of  $CO$  as a function of position across the cloud at steady-state (at a time larger than  $\sim 3 \times 10^6$  years in this case). The solid curve is for the no-diffusion case, the dashed curve is for  $K = 10^{23} \text{ cm}^2 \text{ s}^{-1}$  and the dotted curve is for  $K = 10^{24} \text{ cm}^2 \text{ s}^{-1}$ .



















